Large-Scale Simulations of Shock-Induced Transformations in Gallium, on the Way to Plutonium

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The Modified Embedded Atom-Method (MEAM) [1] applies to metals with greater covalent bonding than the conventional Embedded Atom Method (EAM) [2], which is restricted to nearly-free-electron (simple fcc) metals. MEAM can also describe different crystallographic structures of one element or compound correctly. As a result of the angular bonding terms, semiconductors like Ga [3] and complex elements like Pu can be described reliably.

Shock-induced phase transformations are of principal and programmatic interest and have been investigated in some detail for Fe [4]. Here, we utilize a MEAM potential for Ga [3] to investigate the shock-induced transformation in Ga. The large-scale simulations were performed with the MD code SPaSM (Scalable Parallel Short-range Molecular dynamics) [5, 6, 7] and made use of 256 CPUs of the QSC machine at Los Alamos National Laboratory for 8 hours for each run shown in Fig. 1. Ga has an interesting phase diagram with an orthorhombic ground state structure with a significant amount of dimerization (A11, GaI). It also has at least two more solid phases and a melting temperature of about 300 K at zero pressure.

The ongoing work of atomistic large-scale simulations to understand the dynamics of shock-induced plasticity in Ga will pave the way to tackle the even more challenging dynamics of Pu and its alloys.

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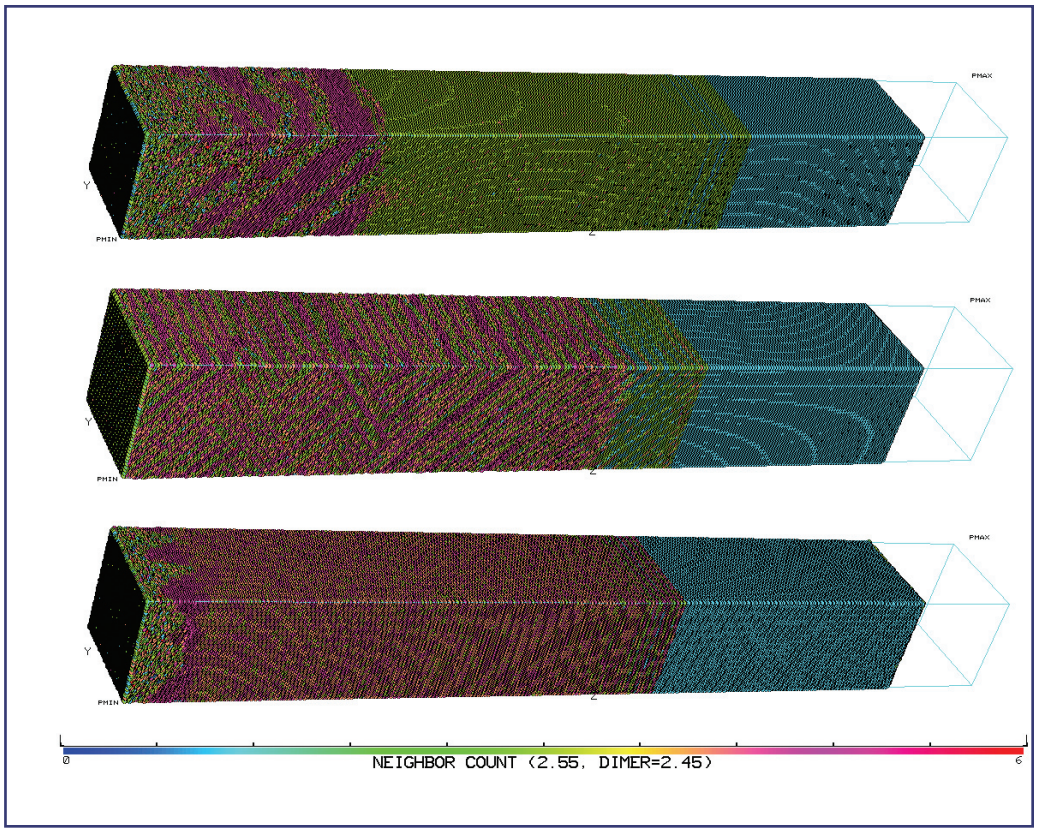

Figure 1—
Samples containing about 2 million Ga atoms (about 17 nm x 17 nm x 140 nm) as modeled by a MEAM potential after 25.5 ps. Piston velocity is 600 m/s and the shock wave traveled from the left to right. Different crystallographic shock directions ([100], [010], [001] top to bottom) result in differences in the resulting structures behind the shock front. The atoms are colored according to the number of neighbors within a radius (2.55 Angstrom) that is slightly larger than the dimer distances of the A11 ground structure (2.45 Angstrom). In all three cases the unshocked A11 structure is blue (neighbor count = 1). In the [100] and [010] cases the following elastic wave is green and the slower plastic wave is marked by the red color. In the case where the shock travels along the dimer direction, i.e., [001] the uniaxially compressed region has more neighbors as in the two other cases and is thus marked by the red color as well; here the plastic front has just started to develop at the very left side.